Markov chain Monte Carlo methods for the regular two-level fractional factorial designs and cut ideals

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Abstract

It is known that a Markov basis of the binary graph model of a graph G corresponds to a set of binomial generators of cut ideals $I_{\widehat{G}}$ of the suspension $\widehat{G}$ of G. In this paper, we give another application of cut ideals to statistics. We show that a set of binomial generators of cut ideals is a Markov basis of some regular two-level fractional factorial design. As application, we give a Markov basis of degree 2 for designs defined by at most two relations.

Introduction

Application of Gröbner bases theory to designed experiments is one of the main branches in a relatively new field in statistics, called *computational algebraic statistics*. The first work in this branch is given by Pistone and Wynn ([20]). In this paper, they presented a method to handle fractional factorial designs algebraically by defining *design ideals*. As one of the merits to consider design ideals, confounding relations between the factor effects can be generalized naturally from regular to non-regular designs and can be expressed concisely by the Gröbner bases theory. See [20] or [12] for details. After this work, various algebraic techniques based on the Gröbner bases theory are applied to the problems of designed experiments both by algebraists and statisticians. For example, an indicator function defined in [11] is a valuable tool to characterize non-regular fractional factorial designs.

On the other hand, there is another main branch in the field of computational algebraic statistics. In this branch, a key notion is a *Markov basis*, which is defined by Diaconis and Sturmfels ([7]). In this work, they established a procedure for sampling from discrete conditional distributions by constructing a connected Markov chain on a given sample space. Since this work many papers are given considering Markov bases for various statistical models, especially for the hierarchical models of multi-dimensional contingency tables. Intensive results on the structure of Markov bases for various statistical models are given in [3].

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The arguments in this paper relates to both of the two branches mentioned above. In fact, the motivation of this paper is of interest to investigate statistical problems which are related to both designed experiments and Markov bases. This paper is based on the first works with this motivation, [5] and [4]. In these works, Markov chain Monte Calro methods for testing factor effects are discussed, when observations are discrete and are given in the two-level or three-level regular fractional factorial designs. As one of the contributions of these works, the relation between the statistical models for the regular fractional factorial designs and contingency tables is considered through Markov bases. As a consequence, to investigate the Markov bases arising in the problems of designed experiments, we can refer to the known results on the corresponding models for the contingency tables. For example, we see that the Markov basis for the main effect models of the regular 2^{5-2}_{III} design given by the defining relation $\mathbf{ABD} = \mathbf{ACE} = \mathbf{I}$ is constructed only by the square-free degree 2 elements ([5]). This is because the corresponding model in the contingency tables is the conditional independence model in the $2 \times 2 \times 2$ table. Note that the conditional independence model in the three-way contingency table is an example of decomposable models and we know the fact that a minimal Markov basis for this class of models can be constructed only by square-free degree 2 elements. See [9] for detail.

In this paper, following the Markov chain Monte Carlo approach in the designed experiments by [5] and [4], we give a new results on the correspondence between the regular two-level design and the algebraic concept, namely *cut ideals* defined in [21]. Because the Markov bases are characterized as the generators of well-specified toric ideals and are studied not only by statisticians but also by algebraists, it is valuable to connect statistical models to known class of toric ideals. In this paper, we give a fundamental fact that the generator of cut ideals can be characterized as the Markov bases for the testing problems of log-linear models for the two-level regular fractional factorial designs.

The construction of this paper is as follows. In Section 1 we review Markov chain Monte Carlo approach for testing the fitting of the log-linear models when observations are discrete random variables. The main results of this paper are given in Section 2. We show how to relate cut ideals to the fractional factorial designs and give the main theorem. In Section 3, we apply known results on the cut ideals to the regular fractional factorial designs.

1 Markov chain Monte Carlo method for regular two-level fractional factorial designs

In this section we introduce Markov chain Monte Carlo methods for testing the fitting of the log-linear models for regular two-level fractional factorial designs with count observations. Suppose we have nonnegative integer observations for each run of a regular fractional design. For simplicity, we also suppose that the observations are counts of some events and only one observation is obtained for each run. This is natural for the settings of Poisson sampling scheme, since the set of the totals for each run is the sufficient statistics for the parameters. We begin with an example.

Table 1: Design and number of defects y for the wave-solder experiment

	Factor							y		
Run	**A**	**B**	**C**	**D**	**E**	**F**	**G**	1	2	3
1	1	1	1	1	1	1	1	13	30	26
2	1	1	1	2	2	2	2	4	16	11
3	1	1	2	1	1	2	2	20	15	20
4	1	1	2	2	2	1	1	42	43	64
5	1	2	1	1	2	1	2	14	15	17
6	1	2	1	2	1	2	1	10	17	16
7	1	2	2	1	2	2	1	36	29	53
8	1	2	2	2	1	1	2	5	9	16
9	2	1	1	1	2	2	1	29	0	14
10	2	1	1	2	1	1	2	10	26	9
11	2	1	2	1	2	1	2	28	173	19
12	2	1	2	2	1	2	1	100	129	151
13	2	2	1	1	1	2	2	11	15	11
14	2	2	1	2	2	1	1	17	2	17
15	2	2	2	1	1	1	1	53	70	89
16	2	2	2	2	2	2	2	23	22	7

Example 1.1 (Wave-soldering experiment)**.** Table 1.1 is a 1/8 fraction of a full factorial design (i.e., a 2^{7-3} fractional factorial design) defined from the defining relation

$$\mathbf{ABDE} = \mathbf{ACDF} = \mathbf{BCDG} = \mathbf{I}, \tag{1}$$

and response data analyzed in [6] and reanalyzed in [14]. In Table 1.1, the observation y is the number of defects arising in a wave-soldering process in attaching components to an electronic circuit card. In Chapter 7 of [6], he considered seven factors of a wave-soldering process: (A) prebake condition, (B) flux density, (C) conveyer speed, (D) preheat condition, (E) cooling time, (F) ultrasonic solder agitator and (G) solder temperature, each at two levels with three boards from each run being assessed for defects. The aim of this experiment is to decide which levels for each factors are desirable to reduce solder defects.

Because we only consider designs with a single observation for each run in this paper, we focus on the totals for each run in Table 1.1. We also ignore the second observation in run 11, which is an obvious outlier as pointed out in [14]. Therefore the weighted total of run 11 is $(28 + 19) \times 3/2 = 70.5 \simeq 71$. By replacing 2 by -1 in Table 1.1, we rewrite

$k \times p$ design matrix as D, where each element is $+1$ or -1. Consequently, we have

$$D = \begin{pmatrix} +1 & +1 & +1 & +1 & +1 & +1 & +1 \\ +1 & +1 & +1 & -1 & -1 & -1 & -1 \\ +1 & +1 & -1 & +1 & +1 & -1 & -1 \\ +1 & +1 & -1 & -1 & -1 & +1 & +1 \\ +1 & -1 & +1 & +1 & -1 & +1 & -1 \\ +1 & -1 & +1 & -1 & +1 & -1 & +1 \\ +1 & -1 & -1 & +1 & -1 & -1 & +1 \\ +1 & -1 & -1 & -1 & +1 & +1 & -1 \\ -1 & +1 & +1 & +1 & -1 & -1 & +1 \\ -1 & +1 & +1 & -1 & +1 & +1 & -1 \\ -1 & +1 & -1 & +1 & -1 & +1 & -1 \\ -1 & +1 & -1 & -1 & +1 & -1 & +1 \\ -1 & -1 & +1 & +1 & +1 & -1 & -1 \\ -1 & -1 & +1 & -1 & -1 & +1 & +1 \\ -1 & -1 & -1 & +1 & +1 & +1 & +1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 69 \\ 31 \\ 55 \\ 149 \\ 46 \\ 43 \\ 118 \\ 30 \\ 43 \\ 45 \\ 71 \\ 380 \\ 37 \\ 36 \\ 212 \\ 52 \end{pmatrix}.$$

In this paper, we consider designs of p factors with two-level. We write the observations as $\mathbf{y} = (y_1, \ldots, y_k)'$, where k is the run size and $'$ denotes the transpose. Write the design matrix $D = (d_{ij})$, where $d_{ij} \in \{-1, 1\}$ is the level of the j-th factor in the i-th run for $i = 1, \ldots, k, j = 1, \ldots, p$.

In this case it is natural to consider the Poisson distribution as the sampling model, in the framework of generalized linear models ([17]). The observations $\mathbf{y}$ are realizations from k Poisson random variables $Y_1, \ldots, Y_k$, which are mutually independently distributed with the mean parameter $\mu_i = E(Y_i), i = 1, \ldots, k$. We call the log-linear model written by

$$\log \mu_i = \beta_0 + \beta_i d_{i1} + \cdots + \beta_p d_{ip}, \ i = 1, \ldots, k \tag{2}$$

as the main effect model in this paper. The equivalent model in the matrix form is

$$\begin{pmatrix} \log \mu_1 \\ \vdots \\ \log \mu_k \end{pmatrix} = M\beta,$$

where $\beta = (\beta_0, \beta_1, \ldots, \beta_p)'$ and

$$M = \begin{pmatrix} 1 & & \\ \vdots & & D \\ 1 & & \end{pmatrix}. \tag{3}$$

We call the $k \times (p + 1)$ matrix M a *model matrix* of the main effect model. The interpretation of the parameter β_j in (2) is the parameter contrast for the main effect of the j-th factor. Following the arguments of [5], we can also consider the models including various interaction effects. In this paper, we first describe our methods for the main effect models and will consider how to treat interaction effects afterward.

To judge the fitting of the main effect model (2), we can perform various goodness-of-fit tests. In the goodness-of-fit tests, the main effect model (2) is treated as the null model, whereas the saturated model is treated as the alternative model. Under the null model (2), β is the nuisance parameter and the sufficient statistic for β is given by $M'\mathbf{y} = (\sum_{i=1}^k y_i, \sum_{i=1}^k d_{i1}y_i, \ldots, \sum_{i=1}^k d_{ip}y_i)'$. Then the conditional distribution of $\mathbf{y}$ given the sufficient statistics is written as

$$f(\mathbf{y} \mid M'\mathbf{y} = M'\mathbf{y}^o) = \frac{1}{C(M'\mathbf{y}^o)} \prod_{i=1}^k \frac{1}{y_i!}, \tag{4}$$

where $\mathbf{y}^o$ is the observation count vector and $C(M'\mathbf{y}^o)$ is the normalizing constant determined from $M'\mathbf{y}^o$ written as

$$C(M'\mathbf{y}^o) = \sum_{\mathbf{y}\in\mathcal{F}(M'\mathbf{y}^o)} \left(\prod_{i=1}^k \frac{1}{y_i!} \right), \tag{5}$$

and

$$\mathcal{F}(M'\mathbf{y}^o) = \{\mathbf{y} \mid M'\mathbf{y} = M'\mathbf{y}^o,\ y_i \text{ is a nonnegative integer for } i = 1, \ldots, k\}. \tag{6}$$

Note that by sufficiency the conditional distribution does not depend on the values of the nuisance parameters.

In this paper we consider various goodness-of-fit tests based on the conditional distribution (4). There are several ways to choose the test statistics. For example, the likelihood ratio statistic

$$T(\mathbf{y}) = G^2(\mathbf{y}) = 2\sum_{i=1}^k y_i \log \frac{y_i}{\hat{\mu}_i} \tag{7}$$

is frequently used, where $\hat{\mu}_i$ is the maximum likelihood estimate for μ_i under the null model (i.e., fitted value). Note that the traditional asymptotic test evaluates the upper probability for the observed value $T(\mathbf{y}^o)$ based on the asymptotic distribution χ^2_{k-p-1}. However, since the fitting of the asymptotic approximation may be sometimes poor, we consider Markov chain Monte Carlo methods to evaluate the p values. Using the conditional distribution (4), the exact p value is written as

$$p = \sum_{\mathbf{y}\in\mathcal{F}(M'\mathbf{y}^o)} f(\mathbf{y} \mid M'\mathbf{y} = M'\mathbf{y}^o)\mathbf{1}(T(\mathbf{y}) \geq T(\mathbf{y}^o)), \tag{8}$$

where

$$\mathbf{1}(T(\mathbf{y}) \geq T(\mathbf{y}^o)) = \begin{cases} 1, & \text{if } T(\mathbf{y}) \geq T(\mathbf{y}^o), \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

Of course, if we can calculate the exact p value of (8) and (9), it is best. Unfortunately, however, an enumeration of all the elements in $\mathcal{F}(M'\mathbf{y}^o)$ and hence the calculation of the normalizing constant $C(M'\mathbf{y}^o)$ is usually computationally infeasible for large sample space. Instead, we consider a Markov chain Monte Carlo method. Note that, as one of the important advantages of Markov chain Monte Carlo method, we need not calculate the normalizing constant (5) to evaluate p values.

To perform the Markov chain Monte Carlo procedure, we have to construct a connected, aperiodic and reversible Markov chain over the conditional sample space (6) with the stationary distribution (4). If such a chain is constructed, we can sample from the chain as $\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(T)}$ after discarding some initial burn-in steps, and evaluate p values as

$$\hat{p} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{1}(T(\mathbf{y}^{(t)}) \geq T(\mathbf{y}^o)).$$

Such a chain can be constructed easily by *Markov basis*. Once a Markov basis is calculated, we can construct a connected, aperiodic and reversible Markov chain over the space (6), which can be modified so that the stationary distribution is the conditional distribution (4) by the Metropolis-Hastings procedure. See [7] and [15] for details.

Markov basis is characterized algebraically as follows. Write indeterminates $x_1, \dots, x_k$ and consider polynomial ring $K[x_1, \dots, x_k]$ for some field K. Consider the integer kernel of the transpose of the model matrix M, $\mathrm{Ker}_{\mathbb{Z}} M'$. For each $\mathbf{b} = (b_1, \dots, b_k)' \in \mathrm{Ker}_{\mathbb{Z}} M'$, define binomial in $K[x_1, \dots, x_k]$ as

$$f_{\mathbf{b}} = \prod_{b_j > 0} x_j^{b_j} - \prod_{b_j < 0} x_j^{-b_j}.$$

Then the binomial ideal in $K[x_1, \dots, x_k]$,

$$I(M') = \langle \{ f_{\mathbf{b}} \mid \mathbf{b} \in \mathrm{Ker}_{\mathbb{Z}} M' \} \rangle ,$$

is called a toric ideal with the configuration M'. Let $\{f_{\mathbf{b}^{(1)}}, \dots, f_{\mathbf{b}^{(s)}}\}$ be any generating set of $I(M')$. Then the set of integer vectors $\{\mathbf{b}^{(1)}, \dots, \mathbf{b}^{(s)}\}$ constitutes a Markov basis. See [7] for detail. To compute a Markov basis for given configuration M', we can rely on various algebraic softwares such as 4ti2 ([1]). See the following example.

Example 1.2 (Wave-soldering experiment, continued)**.** We analyze the data in Table 1.1. The fitted value under the main effect model is calculated as

$$\begin{aligned} \hat{\mu} = (&68.87,\ 19.70,\ 78.85,\ 147.59,\ 12.14,\ 54.77,\ 104.53,\ 54.54, \\ &75.31,\ 39.29,\ 75.00,\ 338.37,\ 27.83,\ 52.09,\ 208.47,\ 59.64)'. \end{aligned}$$

Then the likelihood ratio for the observed data is calculated as $T(\mathbf{y}^o) = G^2(\mathbf{y}^o) = 117.81$ and the corresponding asymptotic p value is less than 0.0001 from the asymptotic distribution χ^2_8. This result tells us that the null hypothesis is highly significant and is rejected, i.e., the existence of some interaction effects is suggested. To evaluate the p value by Markov chain Monte Carlo method, we have to calculate a Markov basis first. If we use 4ti2, we prepare the data file (configuration M') as

```
8 16
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1  1  1  1 -1 -1 -1 -1 -1 -1 -1 -1
 1  1  1  1 -1 -1 -1 -1  1  1  1  1 -1 -1 -1 -1
 1  1 -1 -1  1  1 -1 -1  1  1 -1 -1  1  1 -1 -1
```

```
 1 -1  1 -1  1 -1  1 -1  1 -1  1 -1  1 -1  1 -1
 1 -1  1 -1 -1  1 -1  1 -1  1 -1  1  1 -1  1 -1
 1 -1 -1  1  1 -1 -1  1 -1  1  1 -1 -1  1  1 -1
 1 -1 -1  1 -1  1  1 -1  1 -1 -1  1 -1  1  1 -1
```

and run the command `markov`. Then we have a minimal Markov basis with 77 elements as follows.

```
77 16
 0  0  0  0  0  0  0  0  1  1 -1 -1 -1 -1  1  1
 0  0  0  0  0  1 -1  0  1  0  0 -1 -1 -1  1  1
 0  0  0  0  0  1  0 -1  0  1  0 -1 -1 -1  1  1
 0  0  0  0  1  0 -1  0  1  0 -1  0 -1 -1  1  1
 0  0  0  0  1  0  0 -1  0  1 -1  0 -1 -1  1  1
 0  0  0  0  1  1 -1 -1  0  0  0  0 -1 -1  1  1
 0  0  0  1  0  0 -1  0  1  0 -1 -1  0 -1  1  1
.....
```

Using this Markov basis, we can evaluate p value by Markov chain Monte Carlo method. After $50,000$ burn-in-steps from $\mathbf{y}^o$ itself as the initial state, we sample $100,000$ Monte Carlo sample by Metropolis-Hasting algorithm, which yields $\hat{p} = 0.0000$ again. Figure 1 is a histogram of the Monte Carlo sampling of the likelihood ratio statistic under the main effect model, along with the corresponding asymptotic distribution χ^2_8.

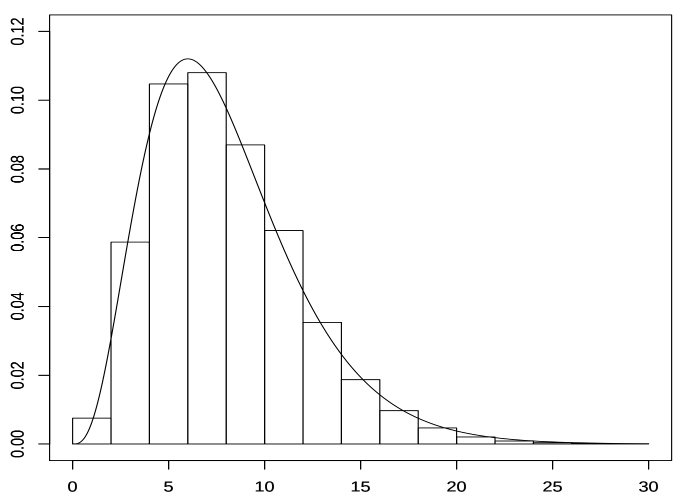


Figure 1: Asymptotic and Monte Carlo estimated distribution of likelihood ratio

If the fitting of the main effect model is poor, or we have some prior knowledge on the existence of interaction effects, we consider the models including interaction effects.

The models including the interaction effects are also described by the model matrix. The modeling method presented in [5] is as follows. If we want to consider the models including interaction effects, add columns to the model matrix of the main effect model (3) so that the corresponding parameter can be interpreted as the parameter contrast for the additional interaction effect. We describe this point by the previous example. See [5] for details.

Example 1.3 (Wave-soldering experiment, continued)**.** As is pointed out in [14], the existence of some interaction effects is suggested for the data in Table 1.1. In [14], the model including 2 two-factor interaction effects, $\mathbf{A} \times \mathbf{C}$ and $\mathbf{B} \times \mathbf{D}$ is considered. Here we call this model as M_2 model. The model matrix of the M_2 model is constructed by adding two columns,

$$\begin{pmatrix} 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \end{pmatrix}'$$

to the model matrix of the main effect model. Note that the above two columns are the element-wise product of the (first, third) columns and the (second, fourth) columns of D, respectively. Using this model matrix (or configuration matrix as its transpose), we can investigate the fitting of the M_2 model in the similar way. The fitted value under the M_2 model is

$$\begin{aligned}\hat{\mu} = (&64.53,\ 47.25,\ 53.15,\ 151.08,\ 30.43,\ 46.79,\ 115.24,\ 32.53,\\ &49.42,\ 46.13,\ 70.90,\ 360.54,\ 35.19,\ 30.26,\ 232.14,\ 51.42)'.\end{aligned}$$

Then the likelihood ratio for the observed data is calculated as $T(\mathbf{y}^o) = G^2(\mathbf{y}^o) = 19.0927$ and the corresponding asymptotic p value is 0.00401 from the asymptotic distribution χ^2_6. Though this result still suggests the significantly poor fitting of the M_2 model, much larger p value and much smaller likelihood ratio than those of the main effect model tell us that M_2 model is much better than the main effect model. We have the Markov chain Monte Carlo estimate of p value as $\hat{p} = 0.0031$ from $100,000$ Monte Calro sample after $50,000$ burn-in-steps.

An important point here is that the model matrix for the models with interaction effects constructed in this way is equivalent to the model matrix for the main effect model for some regular fractional factorial design of resolution III or more. For example, the model matrix for the M_2 model in Example 1.3 is equivalent to the main effect model for the 2^{9-5} fractional factorial design defined from

$$\mathbf{ABDE} = \mathbf{ACDF} = \mathbf{BCDG} = \mathbf{ACH} = \mathbf{BDJ} = \mathbf{I}.$$

This relation is given by adding $\mathbf{H} = \mathbf{AC}$ and $\mathbf{J} = \mathbf{BD}$ to (1), as if there exists two additional factors $\mathbf{H}$ and $\mathbf{J}$ in Table 1.1. In this paper, we consider the relation between the model matrix and the cut ideals. From the above considerations, we can restrict our attentions to the main effect models to consider the relations to the cut ideals. We give the relation in Section 2.2. We will consider the models including interaction effects again in Section 2.3 to consider the relation from the practical viewpoint.

2 Two-level regular fractional factorial designs and cut ideals

In this section, we show that a cut ideal for a finite connected graph can be characterized as the toric ideal $I(M')$ for a model matrix of the main effect model for some regular two-level fractional factorial designs.

2.1 Cut ideals

We start with the definition of the cut ideal. Consider a connected finite graph $G = (V, E)$. We also consider unordered partitions $A|B$ of the vertex set V. Let $\mathcal{P}(V)$ be the set of the unordered partitions of V, i.e.,

$$\mathcal{P}(V) = \{A|B \mid A \cup B = V,\ A \cap B = \emptyset\}.$$

We introduce the sets of indeterminates $\{s_{ij} \mid \{i,j\} \in E\}$, $\{t_{ij} \mid \{i,j\} \in E\}$ and $\{q_{A|B} \mid A|B \in \mathcal{P}(V)\}$. Let

$$\begin{aligned} K[\mathbf{q}] &= K[q_{A|B} \mid A|B \in \mathcal{P}(V)], \\ K[\mathbf{s},\mathbf{t}] &= K[s_{ij}, t_{ij} \mid \{i,j\} \in E] \end{aligned}$$

be polynomial rings over a field K. For each partition $A|B \in \mathcal{P}(V)$, we define a subset $\mathrm{Cut}(A|B)$ of the edge set E as

$$\mathrm{Cut}(A|B) = \{\{i,j\} \in E \mid i \in A, j \in B \text{ or } i \in B, j \in A\}.$$

Define homomorphism of polynomial rings as

$$\phi_G :\ K[\mathbf{q}] \to K[\mathbf{s},\mathbf{t}], \quad q_{A|B} \mapsto \prod_{\{i,j\} \in \mathrm{Cut}(A|B)} s_{ij} \cdot \prod_{\{i,j\} \in E \setminus \mathrm{Cut}(A|B)} t_{ij}. \tag{10}$$

We may think of $\mathbf{s}$ and $\mathbf{t}$ as abbreviations for "separated" and "together", respectively. Then the cut ideal of the graph G is defined as $I_G = \mathrm{Ker}(\phi_G)$. We also use the following two examples given in [21].

Example 2.1 (Complete graph on four vertices)**.** Let $G = K_4$ be the complete graph on four vertices $V = \{1,2,3,4\}$. Then the edge set is $E = \{12, 13, 14, 23, 24, 34\}$. The map ϕ_{K_4} is specified by

$$\begin{array}{rcl} q_{\emptyset|1234} & \mapsto & t_{12}t_{13}t_{14}t_{23}t_{24}t_{34} \\ q_{1|234} & \mapsto & s_{12}s_{13}s_{14}t_{23}t_{24}t_{34} \\ q_{2|134} & \mapsto & s_{12}t_{13}t_{14}s_{23}s_{24}t_{34} \\ q_{3|124} & \mapsto & t_{12}s_{13}t_{14}s_{23}t_{24}s_{34} \\ q_{4|123} & \mapsto & t_{12}t_{13}s_{14}t_{23}s_{24}s_{34} \\ q_{12|34} & \mapsto & t_{12}s_{13}s_{14}s_{23}s_{24}t_{34} \\ q_{13|24} & \mapsto & s_{12}t_{13}s_{14}s_{23}t_{24}s_{34} \\ q_{14|23} & \mapsto & s_{12}s_{13}t_{14}t_{23}s_{24}s_{34}. \end{array}$$

In this case, the cut ideal is a principal ideal given by

$$I_{K_4} = \left\langle q_{\emptyset|1234}q_{12|34}q_{13|24}q_{14|23} - q_{1|234}q_{2|134}q_{3|124}q_{4|123} \right\rangle.$$

Example 2.2 (4-cycle)**.** Let $G = C_4$ be the 4-cycle with

$$V = \{1,2,3,4\},\ E = \{12,23,34,14\}.$$

The map ϕ_{C_4} is derived from ϕ_{K_4} in Example 2.1 by setting

$$s_{13} = t_{13} = s_{24} = t_{24} = 1$$

as

$$\begin{array}{rcl} q_{\emptyset|1234} & \mapsto & t_{12}t_{14}t_{23}t_{34} \\ q_{1|234} & \mapsto & s_{12}s_{14}t_{23}t_{34} \\ q_{2|134} & \mapsto & s_{12}t_{14}s_{23}t_{34} \\ q_{3|124} & \mapsto & t_{12}t_{14}s_{23}s_{34} \\ q_{4|123} & \mapsto & t_{12}s_{14}t_{23}s_{34} \\ q_{12|34} & \mapsto & t_{12}s_{14}s_{23}t_{34} \\ q_{13|24} & \mapsto & s_{12}s_{14}s_{23}s_{34} \\ q_{14|23} & \mapsto & s_{12}t_{14}t_{23}s_{34}. \end{array}$$

In this case, the cut ideal is given by

$$I_{C_4} = \left\langle q_{\emptyset|1234}q_{13|24} - q_{1|234}q_{3|124},\ q_{\emptyset|1234}q_{13|24} - q_{2|134}q_{4|123},\ q_{\emptyset|1234}q_{13|24} - q_{12|34}q_{14|23} \right\rangle.$$

Now we relates the cut ideals to the regular two-level fractional factorial designs. We express the map ϕ_G by $2^{|V|-1} \times 2|E|$ matrix $H = \{h_{A|B,e}\}$ where each row of H represents $A|B \in \mathcal{P}(V)$ and each two columns of H represents E as

$$h_{A|B,e} = \begin{cases} (1,0) & \text{if } e \in E \setminus \mathrm{Cut}(A|B) \\ (0,1) & \text{if } e \in \mathrm{Cut}(A|B). \end{cases}$$

Note that there are $|\mathcal{P}(V)| = 2^{|V|-1}$ unordered partitions of V. We also see that each two columns of H correspond to $\mathbf{t}$ and $\mathbf{s}$. Then the cut ideal, the kernel of ϕ_G of (10), is written as the toric ideal of the configuration matrix H'.

Example 2.3 (4-cycle, continued)**.** For the case of $G = C_4$ of Example 2.2, the matrix H can be written as follows.

$$\begin{array}{r|cccccccc|} & t_{12} & s_{12} & t_{14} & s_{14} & t_{23} & s_{23} & t_{34} & s_{34} \\ \hline q_{\emptyset|1234} & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ q_{3|124} & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ q_{4|123} & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ q_{12|34} & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ q_{14|23} & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ q_{2|134} & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ q_{1|234} & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ q_{13|24} & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ \hline \end{array} \qquad (11)$$

The kernel of H' coincides to the kernel of M' of (3) for the two-level design D of $|E|$ factors with $2^{|V|-1}$ runs, where the level of the factor X_e for the run $A|B \in \mathcal{P}(V)$ is given by the following map:

$$\begin{array}{rccc} X_e: & \mathcal{P}(V) & \to & \{+1,-1\} \\ & \cup\!\!\!\!\mid & & \cup\!\!\!\!\mid \\ & A|B & \mapsto & \begin{cases} +1 & \text{if } e \in E \setminus \mathrm{Cut}(A|B) \\ -1 & \text{if } e \in \mathrm{Cut}(A|B) \end{cases} \end{array} \qquad (12)$$

Example 2.4 (4-cycle, continued)**.** For the case of $G = C_4$, the map X_e of (12) gives the design matrix D as follows.

$$\begin{array}{c} \\ q_{\emptyset|1234} \\ q_{3|124} \\ q_{4|123} \\ q_{12|34} \\ q_{14|23} \\ q_{2|134} \\ q_{1|234} \\ q_{13|24} \end{array} \begin{array}{c} \begin{array}{rrrr} X_{12} & X_{14} & X_{23} & X_{34} \end{array} \\ \boxed{\begin{array}{rrrr} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 \end{array}} \end{array}$$

For this D, it is easily seen that $\mathrm{Ker}(M')$ coincides to $\mathrm{Ker}(H')$ if H is given by (11).

2.2 Regular designs and cut ideals

In Example 2.4, we obtain the toric ideal for the main effect model of the regular two-level fractional factorial designs defined by $X_{12}X_{14}X_{23}X_{34} = 1$ from the the cut ideal of $G = C_4$. In fact, there is a clear relation between finite connected graphs G and regular two-level designs D. As we have seen in Example 2.4, the cut ideal for G can be related to the design of $p = |E|$ factors with $k = 2^{|V|-1}$ runs. Since each factor of this design corresponds to the edge E of G, we write each factor X_{ij} for $\{i, j\} \in E$. Since there are 2^p runs in the full factorial design of p factors, the design obtained from G by the relation (12) is a $2^{|V|-1-p}$ fraction of the full factorial design of p factors. We show this fraction is specified as the regular fractional factorial designs.

Let $G = (V, E)$ be a finite connected graph with the edge set $E = \{e_1, \ldots, e_p\}$. Then, the *cycle space* $\mathcal{C}(G)$ of G is a subspace of $\mathbb{F}_2^{|E|}$ spanned by

$$\left\{ \mathbf{e}_{i_1} + \cdots + \mathbf{e}_{i_r} \in \mathbb{F}_2^{|E|} \;\middle|\; (e_{i_1}, \ldots, e_{i_r}) \text{ is a cycle of } G \right\},$$

where $\mathbf{e}_j$ is the jth coordinate vector of $\mathbb{F}_2^{|E|}$. On the other hand, the *cut space* $\mathcal{C}^*(G)$ of G is a subspace of $\mathbb{F}_2^{|E|}$ defined by

$$\mathcal{C}^*(G) = \left\{ \sum_{e_j \in \mathrm{Cut}(A|B)} \mathbf{e}_j \in \mathbb{F}_2^{|E|} \;\middle|\; A|B \in \mathcal{P}(V) \right\}.$$

Fix a spanning tree T of G. For each $e \in E \setminus T$, the set $T \cup \{e\}$ has exactly one cycle C_e of G. Such a cycle C_e is called a *fundamental cycle* of G. Since T has $|V| - 1$ edges, there are $|E| - |V| + 1$ edges in $E \setminus T$. It then follows that there exists $|E| - |V| + 1$ fundamental cycles in G. The following proposition is known in graph theory [8]:

Proposition 2.5. *Let $G = (V, E)$ be a finite connected graph. Then, we have the following:*

(i) $\mathcal{C}^*(G) = \mathcal{C}(G)^\perp \left(= \left\{ \mathbf{v} \in \mathbb{F}_2^{|E|} \;\middle|\; \mathbf{v} \cdot \mathbf{u} = 0 \textit{ for all } \mathbf{u} \in \mathcal{C}(G) \right\} \right);$

(ii) *Given spanning tree of G, the cycle space $\mathcal{C}(G)$ is spanned by*

$$\left\{ \mathbf{e}_{i_1} + \cdots + \mathbf{e}_{i_r} \in \mathbb{F}_2^{|E|} \;\middle|\; (e_{i_1}, \ldots, e_{i_r}) \text{ is a fundamental cycle of } G \right\};$$

(iii) $\dim \mathcal{C}(G) = |E| - |V| + 1$ *and* $\dim \mathcal{C}^*(G) = |V| - 1$.

By Proposition 2.5, we have the following:

Theorem 2.6. *Let $G = (V, E)$ be a finite connected graph and let D be the design matrix of $|E|$ factors with $2^{|V|-1}$ runs defined by (12). Then D is a regular fractional factorial design with all relations*

$$X_{e_{i_1}}(A|B) X_{e_{i_2}}(A|B) \cdots X_{e_{i_m}}(A|B) = 1, \tag{13}$$

where $(e_{i_1}, \ldots, e_{i_m})$ is a fundamental cycle of G.

Proof. The equation (13) is equivalent to the equation

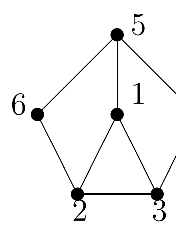
$$(\mathbf{e}_{i_1} + \cdots + \mathbf{e}_{i_m}) \cdot \left(\sum_{e_j \in \mathrm{Cut}(A|B)} \mathbf{e}_j \right) = 0$$

in $\mathbb{F}_2^{|E|}$. Thus, the assertion follows from (i) and (ii) of Proposition 2.5. $\square$

It may be a helpful to see a typical example.

Example 2.7. Consider $G = (V, E)$ given by

$$V = \{1, 2, 3, 4, 5, 6\}, \; E = \{12, 13, 23, 34, 45, 56, 26\}.$$



From (13), we see that G corresponds to 2^{7-3} design with

$$X_{12}X_{13}X_{23} = X_{13}X_{34}X_{45}X_{15} = X_{12}X_{26}X_{56}X_{15} = 1.$$

Note that the relations corresponding the dependent cycles such as $\{23, 34, 45, 56, 26\}$ can be derived as

$$X_{23}X_{34}X_{45}X_{56}X_{26} = (X_{12}X_{13}X_{23})(X_{13}X_{34}X_{45}X_{15})(X_{12}X_{26}X_{56}X_{15}) = 1.$$

Theorem 2.6 shows the relation of the cut ideals and regular two-level fractional factorial designs. For a given connected finite graph, we can consider corresponding regular two-level fractional factorial designs from Theorem 2.6. Unfortunately, however, the converse does not always hold. For given regular two-level fractional factorial designs (strictly, we should say that "for given designs and *models*", which we consider in Section 2.3), it does not always exist corresponding connected finite graphs.

Proposition 2.8. *If a 2^{p-q} design corresponds to a finite graph by the relation (12), then we have $p \leq \binom{p-q+1}{2}$.*

Proof. Corresponding connected graphs $G = (V, E)$ does not exist because $|E| = p$ and $|V| = p - q + 1$ must be satisfied if it exists. (There are $\binom{p-q+1}{2}$ edges in K_{p-q+1}.) $\square$

Thus, obvious counterexamples for the converse are given since some regular 2^{p-q} designs satisfy $\binom{p-q+1}{2} < p$ (for example, $(p, q) = (5, 3), (5, 4), (6, 4), (6, 5)$ and so on). On the other hand, a necessary condition related with the resolution is as follows.

Proposition 2.9. *If a 2^{p-q} design of resolution* IV *or more corresponds to a finite graph by the relation (12), then we have $p \leq \lfloor (p-q+1)^2/4 \rfloor$.*

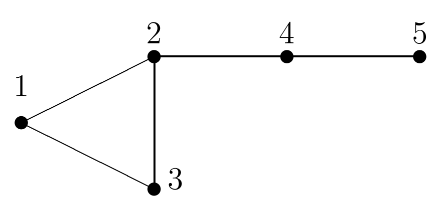
Proof. Mantel's theorem in graph theory says that the number of edges in triangle-free graph with n vertices is at most $\lfloor n^2/4 \rfloor$. $\square$

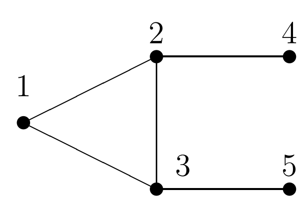
If the resolution of a design is V or more, then similar results are obtained by the results in [13]. From these considerations, an important question arises.

Question 2.10. *Characterize regular two-level fractional factorial designs that can correspond to a finite graph by the relation (12).*

A complete answer to this question is not yet obtained at present. We give results for 8 runs and 16 runs designs in Section 2.3. We present several fundamental characterizations in the rest of this section. Note that the above correspondence is not one-to-one even if it exists. In fact, for any finite connected graph G, we can specify a design D uniquely by (13). However, for a given design G, we can consider several graphs satisfying the relation (13) if it exists.

Example 2.11 (2^{5-1} design with $X_{12}X_{13}X_{23} = 1$ of 5 factors)**.** Consider 2^{5-1} fractional factorial design $X_{12}X_{13}X_{23} = 1$ of 5 factors, or, $\mathbf{ABC} = \mathbf{I}$ in the convention of designed experiment literature. There are several corresponding graphs that give this design such as follows.

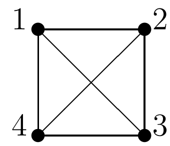




Later, we will be able to understand this by Proposition 3.1. (Both of two graphs are 0-sum of the same pair of graphs.)

Now we show two important special cases, designs corresponding to complete graphs and trees.

Example 2.12 (Complete graph on four vertices (continued))**.** Let $G = K_4$ be the complete graph on four vertices $V = \{1, 2, 3, 4\}$ in Example 2.1.



From (13), we have the following regular 2^{6-3} fractional factorial design.

	X_{12}	X_{13}	X_{14}	X_{23}	X_{24}	X_{34}
$q_{\emptyset\|1234}$	1	1	1	1	1	1
$q_{3\|124}$	1	−1	1	−1	1	−1
$q_{4\|123}$	1	1	−1	1	−1	−1
$q_{12\|34}$	1	−1	−1	−1	−1	1
$q_{14\|23}$	−1	−1	1	1	−1	−1
$q_{2\|134}$	−1	1	1	−1	−1	1
$q_{1\|234}$	−1	−1	−1	1	1	1
$q_{13\|24}$	−1	1	−1	−1	1	−1

The defining relation of this design is

$$X_{12}X_{13}X_{23} = X_{12}X_{14}X_{24} = X_{13}X_{14}X_{34} = 1,$$

where the three terms $X_{12}X_{13}X_{23}, X_{12}X_{14}X_{24}, X_{13}X_{14}X_{34}$ correspond to the independent cycle of K_4.

Generalizing Example 2.12, we summarize the following important cases.

Corollary 2.13. *Let $G = K_n$ be the complete graph on $|V| = n$ vertices. Then, G is specified as the regular $2^{c_1-c_2}$ fractional factorial design of c_1 two-level factors by (13), where*

$$c_1 = \binom{n}{2}, \quad c_2 = \binom{n-1}{2}.$$

The defining relation of this design is written as $X_{1i}X_{1j}X_{ij} = 1$ for any pair (i, j) with $2 \leq i < j \leq n$.

Another important case is as follows.

Corollary 2.14. *Any spanning tree $G = (V, E)$ is specified as the full factorial design of $|V| - 1$ two-level factors by (13).*

2.3 Models for the designs with 8 runs and 16 runs

It seems very difficult to answer Question 2.10 in general. As special cases, we show that 2^{p-1} and 2^{p-2} fractional factorial designs can relate to graphs from algebraic theories in Section 3. As another approach, we investigate all the practical models arising in the two-level fractional factorial designs with 8 runs and 16 runs. In Section 2.3, we consider models with interaction effects to classify the cases arising in applications.

First we consider models for the designs with 8 runs. Among the regular designs with 8 runs, the most frequently used designs are listed in Table 2. We ignore 2^{7-4}_{III} design in

Table 2: 2^{p-q} fractional factorial designs with 8 runs ($p-q=3$)

Number of factors p	Resolution	Design Generators
4	IV	$\mathbf{D} = \mathbf{ABC}$
5	III	$\mathbf{D} = \mathbf{AB},\ \mathbf{E} = \mathbf{AC}$
6	III	$\mathbf{D} = \mathbf{AB},\ \mathbf{E} = \mathbf{AC},\ \mathbf{F} = \mathbf{BC}$
7	III	$\mathbf{D} = \mathbf{AB},\ \mathbf{E} = \mathbf{AC},\ \mathbf{F} = \mathbf{BC}, \mathbf{G} = \mathbf{ABC}$

Table 2 since the main effect model is saturated and cannot be tested in our method. For the other 3 designs, $2^{4-1}_{\mathrm{IV}}, 2^{5-2}_{\mathrm{III}}$ and 2^{6-3}_{III} designs, we consider models to be tested.

For 2^{4-1}_{IV} design of $\mathbf{ABCD} = \mathbf{I}$, we can consider 3 models as follows.

- Main effect model:
  We write it as $\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}$.

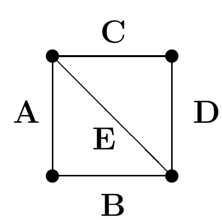
- Models with all the main effects and 1 two-factor interaction effect:
  Without loss of generality, we consider $\mathbf{A} \times \mathbf{B}$ as the interaction effect. We write it as $\mathbf{AB}/\mathbf{C}/\mathbf{D}$.

- Models with all the main effects and 2 two-factor interaction effects:
  Note that we cannot consider models including, say, $\mathbf{A} \times \mathbf{B}$ and $\mathbf{C} \times \mathbf{D}$, because they are confounded. Without loss of generality, we consider $\mathbf{A} \times \mathbf{B}$ and $\mathbf{A} \times \mathbf{C}$ as the two interaction effects. We write it as $\mathbf{AB}/\mathbf{AC}/\mathbf{D}$.

Note that we cannot consider models with more than 2 two-factor interactions because there are 8 parameters in the saturated models for the design with 8 runs. For these models, we can construct model matrix and consider existence of corresponding graphs. As we have seen, the model $\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}$ can relate to the 4-cycle. For the model $\mathbf{AB}/\mathbf{C}/\mathbf{D}$, we introduce imaginary factor $\mathbf{E} = \mathbf{AB}$ and consider the main effect model for the 2^{5-2} design defined by

$$\mathbf{ABCD} = \mathbf{ABE}\ (= \mathbf{CDE}) = \mathbf{I}$$

as we have seen in the last of Section 1. This corresponds to the graph with 5 edges as follows.



Similarly, for the model $\mathbf{AB}/\mathbf{AC}/\mathbf{D}$, introducing imaginary factors $\mathbf{E} = \mathbf{AB}$ and $\mathbf{F} = \mathbf{AC}$ and consider the main effect model for the 2^{6-3} design defined by

$$\mathbf{ABCD} = \mathbf{ABE} = \mathbf{ACF} = \mathbf{I},$$

we see the corresponding graph is K_4.

Table 3: Models for the designs in Table 2

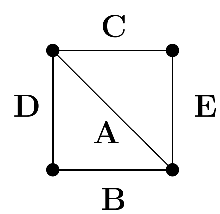
Design	Num. of parameters	Model	Index
2_{IV}^{4-1}	5	$\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}$	[1]
	6	$\mathbf{AB}/\mathbf{C}/\mathbf{D}$	[2]
	7	$\mathbf{AB}/\mathbf{AC}/\mathbf{D}$	[3]
2_{III}^{5-2}	6	$\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}/\mathbf{E}$	[4]
	7	$\mathbf{A}/\mathbf{BC}/\mathbf{D}/\mathbf{E}$	[5]
2_{III}^{6-3}	7	$\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}/\mathbf{E}/\mathbf{F}$	[6]

For 2_{III}^{5-2} design of $\mathbf{D} = \mathbf{AB}, \mathbf{E} = \mathbf{AC}$, we can consider only one additional interaction effect to the main effect model. Therefore there are the following 2 models to be considered.

- Main effect model:
  We write it as $\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}/\mathbf{E}$.

- Models with all the main effects and 1 two-factor interaction effect:
  Note that we cannot consider models including, say, $\mathbf{A} \times \mathbf{B}$, because it is confounded to the main effect of $\mathbf{D}$. Without loss of generality, we consider $\mathbf{B} \times \mathbf{C}$ as the interaction effect, with we write $\mathbf{A}/\mathbf{BC}/\mathbf{D}/\mathbf{E}$.

For these models, we can construct model matrix and consider existence of corresponding graphs. The model $\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}/\mathbf{E}$ can relate to the graph as follows.



We see the model $\mathbf{A}/\mathbf{BC}/\mathbf{D}/\mathbf{E}$ can relate to K_4 by introducing imaginary factor $\mathbf{F} = \mathbf{BC}$.

Finally, for 2_{III}^{6-3} design of $\mathbf{D} = \mathbf{AB}, \mathbf{E} = \mathbf{AC}, \mathbf{F} = \mathbf{BC}$, only the main effect model can be considered, which can be relate to K_4.

From the above considerations, we have complete classification of all the hierarchical models for the designs with 8 runs in Table 2. We summarize the results in Table 3 and Table 4.

Next we consider models for the designs with 16 runs in a similar way. The most frequently used designs with 16 runs are given Section 4 of [22], which we show in Table 5. For the designs in Table 5, we consider possible models. For the designs with 16 runs, we can test models with less than 16 parameters. However, the models with parameters more than 11 $(= 10 + 1)$ cannot relate to graphs obviously because there are 10 edges in K_5. Therefore we only consider models with at most 11 parameters.

Moreover, we can use the fact that if some model has a corresponding graph, its each submodel also has a corresponding graph. We can confirm this fact by tracing the arguments of imaginary factors reversely. Suppose some model $\mathcal{M}$ with the interaction factor

Table 4: Graphs corresponding to the models in Table 3

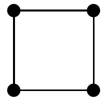
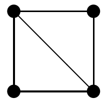
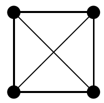
Graph	Models
	[1]
	[2][4]
	[3][5][6]

Table 5: 2^{p-q} fractional factorial designs with 16 runs ($p-q=4$)

Number of factors p	Resolution	Design Generators
5	V	$\mathbf{E} = \mathbf{ABCD}$
6	IV	$\mathbf{E} = \mathbf{ABC}, \mathbf{F} = \mathbf{ABD}$
7	IV	$\mathbf{E} = \mathbf{ABC}, \mathbf{F} = \mathbf{ABD}, \mathbf{G} = \mathbf{ACD}$
8	IV	$\mathbf{E} = \mathbf{ABC}, \mathbf{F} = \mathbf{ABD}, \mathbf{G} = \mathbf{ACD}$
		$\mathbf{H} = \mathbf{BCD}$
9	III	$\mathbf{E} = \mathbf{ABC}, \mathbf{F} = \mathbf{ABD}, \mathbf{G} = \mathbf{ACD}$
		$\mathbf{H} = \mathbf{BCD}, \mathbf{J} = \mathbf{ABCD}$
10	III	$\mathbf{E} = \mathbf{ABC}, \mathbf{F} = \mathbf{ABD}, \mathbf{G} = \mathbf{ACD}$
		$\mathbf{H} = \mathbf{BCD}, \mathbf{J} = \mathbf{ABCD}, \mathbf{K} = \mathbf{CD}$

$\mathbf{A}_1 \times \cdots \times \mathbf{A}_s$ has a corresponding graph G with q dimensional cycle space. The graph G is constructed by introducing imaginary factor $\mathbf{X}$ to consider the cycle $\{\mathbf{X}, \mathbf{A}_1 \ldots, \mathbf{A}_s\}$. It then follows that there exists a spanning tree of G such that $\{\mathbf{X}, \mathbf{A}_1 \ldots, \mathbf{A}_s\}$ is a fundamental cycle. Then, deleting the edge $\mathbf{X}$ yields a graph with $q-1$ dimensional cycle space, which is the corresponding graph of the model $\mathcal{M} \setminus \{\mathbf{A}_1 \times \cdots \times \mathbf{A}_s\}$. In particular, if the main effect model does not have a corresponding graph, all models with interaction effects also do not have a corresponding graph for this design. For the designs of Table 5, we see that the main effect models for 2^{7-3}_{IV}, 2^{8-4}_{IV}, 2^{9-5}_{III} and 2^{10-6}_{III} do not have corresponding graphs. (For example, if a $2^{p-q} = 2^4$ design of resolution IV corresponds to a finite graph by the relation (12), then we have $p \leq \lfloor (4+1)^2/4 \rfloor = 6$ by Proposition 2.9.) Therefore we consider the models for 2^{5-1}_{V} and 2^{6-2}_{IV} designs. The distinct models for these designs are given in Table 6 and Table 7. For the models with no corresponding graphs, only minimal models are included in Table 6 and Table 7. For example, the model $\mathbf{AB}/\mathbf{AC}/\mathbf{AD}/\mathbf{E}$ of the 2^{5-1}_{V}-design does not have a corresponding graph. This is a minimal model in the sense that any submodel of it, i.e., $\mathbf{AB}/\mathbf{AC}/\mathbf{D}/\mathbf{E}$, $\mathbf{AB}/\mathbf{C}/\mathbf{D}/\mathbf{E}$ and $\mathbf{A}/\mathbf{B}/\mathbf{C}/\mathbf{D}/\mathbf{E}$, has a corresponding graph. From the consideration above, we see all models including it, i.e., $\mathbf{AB}/\mathbf{AC}/\mathbf{AD}/\mathbf{AE}$ or $\mathbf{AB}/\mathbf{AC}/\mathbf{BC}/\mathbf{AD}/\mathbf{AE}$, for example, also do not have a corresponding graph.

Table 6: Models for the 2_{V}^{5-1}-design of $\mathbf{E} = \mathbf{ABCD}$

Num. of parameters	Model	Index
6	**A/B/C/D/E**	[5-1]
7	**AB/C/D/E**	[5-2]
8	**AB/AC/D/E**	[5-3]
	AB/CD/E	[5-4]
9	**AB/AC/BD/E**	[5-5]
	AB/AC/DE	[5-6]
	AB/AC/AD/E	(no graph)
	AB/AC/BC/D/E	(no graph)
10	**AB/AC/BD/CE**	[5-7]
	AB/AC/BD/CD	(no graph)
11	**AB/AC/BD/CE/DE**	[5-8]

Table 7: Models for the 2_{IV}^{6-2}-design of $\mathbf{E} = \mathbf{ABC}, \mathbf{F} = \mathbf{ABD}$

Num. of parameters	Model	Index
7	**A/B/C/D/E/F**	[6-1]
8	**AB/C/D/E/F**	[6-2]
	AC/B/D/E/F	[6-3]
9	**AB/AC/D/E/F**	[6-4]
	AB/CD/E/F	[6-5]
10	**AB/AC/AD/E/F**	[6-6]
	AB/AD/BC/E/F	[6-7]
	AB/AC/CD/E/F	[6-8]
	AB/AC/DE/F	[6-9]
	AC/BD/EF	[6-10]
	AB/AC/AE/D/F	(no graph)
	AB/AC/BC/D/E/F	(no graph)
11	**AB/AC/AD/CD/E/F**	[6-11]
	AD/DE/DF/BC	[6-12]
	AD/BC/CF/DF/E	[6-13]
	AC/AD/CD/CF/B/E	(no graph)
	AB/AC/CF/CD/E	(no graph)
	AC/BD/CD/CF/E	(no graph)
	AC/BC/AD/AF/E	(no graph)
	AB/AC/AD/CF/E	(no graph)
	AC/AD/BC/DF/E	(no graph)
	AB/BC/AD/EF	(no graph)
	AD/BC/BD/EF	(no graph)
	AD/BC/BE/DF	(no graph)
	AD/AF/BC/BE	(no graph)

For these models, we can construct model matrix and consider existence of corresponding graphs. The results are shown in Table 8.

3 Application

In this section, we apply known results on cut ideals to the regular two-level fractional factorial designs. First we study fundamental facts on cut ideals appearing in [21]. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs such that $V_1 \cap V_2$ is a clique of both graphs. The new graph $G = G_1 \sharp G_2$ with the vertex set $V = V_1 \cup V_2$ and edge set $E = E_1 \cup E_2$ is called *k-sum* of G_1 and G_2 along $V_1 \cap V_2$ if the cardinality of $V_1 \cap V_2$ is $k + 1$. In this section, we only consider 0, 1, 2-sums. Let

$$\mathbf{f} = \prod_{i=1}^{d} q_{A_i|B_i} - \prod_{i=1}^{d} q_{C_i|D_i}$$

be a binomial in I_{G_1} of degree d. Since $V_1 \cap V_2$ is a clique of G_1 and $|V_1 \cap V_2| \leq 3$, we may assume that $A_i \cap V_1 \cap V_2 = C_i \cap V_1 \cap V_2$ for all i. For any ordered list EF of d partitions of $V_2 \setminus V_1$,

$$EF = (E_1|F_1, E_2|F_2, \ldots, E_d|F_d),$$

we define the binomial in I_G of degree d by

$$\mathbf{f}^{EF} = \prod_{i=1}^{d} q_{A_i \cup E_i | B_i \cup F_i} - \prod_{i=1}^{d} q_{C_i \cup E_i | D_i \cup F_i} \in I_G.$$

If $\mathbf{F}$ is a set of binomials in I_{G_1}, then we define

$$\mathrm{Lift}(\mathbf{F}) = \left\{ \mathbf{f}^{EF} \;\middle|\; \mathbf{f} \in \mathbf{F},\ EF = \{E_i|F_i\}_{i=1}^{\deg \mathbf{f}} \right\}.$$

On the other hand, let $\mathrm{Quad}(G_1, G_2)$ be the set of all quadratic binomials

$$q_{A\cup C_1\cup C_2|B\cup D_1\cup D_2} q_{A\cup E_1\cup E_2|B\cup F_1\cup F_2} - q_{A\cup E_1\cup C_2|B\cup F_1\cup D_2} q_{A\cup C_1\cup E_2|B\cup D_1\cup F_2}$$

where

- $A|B$ is an unordered partition of $V_1 \cap V_2$;
- $C_1|D_1$ and $E_1|F_1$ are ordered partitions of $V_1 \setminus V_2$;
- $C_2|D_2$ and $E_2|F_2$ are ordered partitions of $V_2 \setminus V_1$.

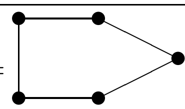
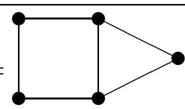
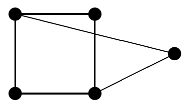
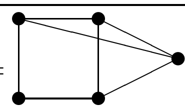
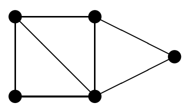
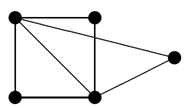
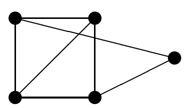
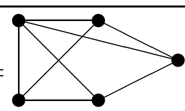
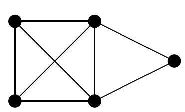
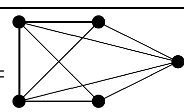
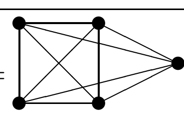
Then, the following is known:

Proposition 3.1 ([21])**.** *Let $G = G_1 \sharp G_2$ be a 0, 1 or 2-sum of G_1 and G_2 and let $\mathbf{F}_i$ be a set of binomial generators of I_{G_i} for $i = 1, 2$. Then I_G is generated by*

$$\mathbf{M} = \mathrm{Lift}(\mathbf{F}_1) \cup \mathrm{Lift}(\mathbf{F}_2) \cup \mathrm{Quad}(G_1, G_2).$$

Moreover, if $\mathbf{F}_i$ is a Gröbner basis of I_{G_i} for $i = 1, 2$, then there exists a monomial order such that $\mathbf{M}$ is a Gröbner basis of I_G.

Table 8: Graphs corresponding to the models in Tables 6 and 7

Graph	Models
$G_1 =$ 	[5-1]
$G_2 =$ 	[5-2]
$G_3 =$ 	[6-1]
$G_4 =$ 	[5-3]
$G_5 =$ 	[5-4]
$G_6 =$ 	[6-2]
$G_7 =$ 	[6-3]
$G_8 =$ 	[5-5]
$G_9 =$ 	[5-6][6-4][6-5]
$G_{10} =$ 	[5-7][6-6][6-7][6-8][6-9][6-19]
$G_{11} =$ 	[5-8][6-11][6-12][6-13]

Example 3.2. The graph G_9 in Table 8 is a 1-sum of the complete graph K_4 and a cycle C_3 of length 3. Since I_{K_4} is a principal ideal in Example 2.1 and I_{C_3} is a zero ideal, I_{G_9} is generated by the binomials of degree 2 and 4. On the other hand, the graph G_{10} in Table 8 is a 2-sum of the complete graphs K_4 and K_4. Thus, $I_{G_{10}}$ is generated by the binomials of degree 2 and 4, too.

A graph G is called a *ring graph* if G is obtained by 0/1-sums of cycles and edges. It is known that ring graphs have no K_4 minor.

Proposition 3.3 ([18])**.** *If G is a ring graph, then I_G has a quadratic Gröbner basis.*

Example 3.4. It is easy to see that the graph G_i in Table 8 is a ring graph if and only if $i \in \{1, 2, 5, 6\}$. Thus the cut ideal I_{G_i} has a quadratic Gröbner basis for $i \in \{1, 2, 5, 6\}$.

Let $e = \{i, j\} \in E$ be an edge of a graph $G = (V, E)$. Then, the new graph $G \setminus e := (V, E \setminus \{e\})$ is called the graph obtained from G by *deleting* e. On the other hand, the new graph G/e obtained by the procedure

(i) Identify the vertices i and j;

(ii) Delete the multiple edges that may be created while (i);

is called the graph obtained from G by *contracting* e. A graph H is said to be a *minor* of G if it can be obtained from G by a sequence of deletions and/or contractions of edges (and deletions of vertices). The following theorem is conjectured by Sturmfels–Sullivant [21] and proved by Engström:

Proposition 3.5 ([10])**.** *The toric ideal I_G is generated by quadratic binomials if and only if G has no K_4 minor.*

Example 3.6. It is easy to see that the graph G_i in Table 8 does not have K_4 minor if and only if $i \in \{1, 2, 3, 5, 6\}$. Thus the cut ideal I_{G_i} is generated by quadratic binomials if and only if $i \in \{1, 2, 3, 5, 6\}$.

Let G be a graph with vertex set $V = \{1, \ldots, n\}$ and edge set E. The *suspension* of the graph G is the new graph $\widehat{G}$ whose vertex set equals $V \cup \{n + 1\}$ and whose edge set equals $E \cup \{\{i, n + 1\} \mid i \in V\}$. It is known [21] that the toric ideal of the binary graph model of G equals to the cut ideal $I_{\widehat{G}}$ of $\widehat{G}$.

Proposition 3.7 ([16])**.** *Let $\widehat{G}$ be the suspension of G. Then $I_{\widehat{G}}$ is generated by binomials of degree ≤ 4 if and only if G has no K_4 minor.*

Example 3.8. The graph G_8 in Table 8 is the suspension of a cycle C_4 of length 4. Since C_4 has no K_4 minor, I_{G_8} is generated by the binomials of degree ≤ 4. On the other hand, the graph $G_{11} = K_5$ in Table 8 is the suspension of K_4. Thus, $I_{G_{11}}$ is not generated by the binomials of degree ≤ 4.

We now apply these known results to our problem.

Theorem 3.9. *Let D be a regular fractional factorial design with at most two defining relations. Then there exists a connected graph $G = (V, E)$ such that*

- *D is the design matrix of $|E|$ factors with $2^{|V|-1}$ runs defined by (12).*
- *I_G is generated by quadratic binomials.*

Moreover, if D has exactly one defining relations, then I_G has a quadratic Gröbner basis.

Proof. Let D be a regular 2^{p-1} fractional factorial design with the defining relation

$$\mathbf{A}_1\mathbf{A}_2\cdots\mathbf{A}_r = \mathbf{I}.$$

Let $G = (V, E)$ be a graph on the vertex set $V = \{1, 2, \ldots, p\}$ with the edge set

$$E = \{12, 23, \ldots, (r-1)r, 1r, r(r+1), (r+1)(r+2), \ldots, (p-1)p\}.$$

Then, it is easy to see that D is the design matrix of $|E|$ factors with $2^{|V|-1}$ runs defined by (12). Since G is a ring graph, I_G has a quadratic Gröbner basis by Proposition 3.3.

Let D be a regular 2^{p-2} fractional factorial design with the defining relation

$$\mathbf{A}_1\mathbf{A}_2\cdots\mathbf{A}_r\mathbf{B}_1\mathbf{B}_2\cdots\mathbf{B}_s = \mathbf{B}_1\mathbf{B}_2\cdots\mathbf{B}_s\mathbf{C}_1\mathbf{C}_2\cdots\mathbf{C}_t = \mathbf{I},$$

where $0 \le s \in \mathbb{Z}$ and $1 \le r, t \in \mathbb{Z}$. Let $G = (V, E)$ be the graph in Figure 2. It then

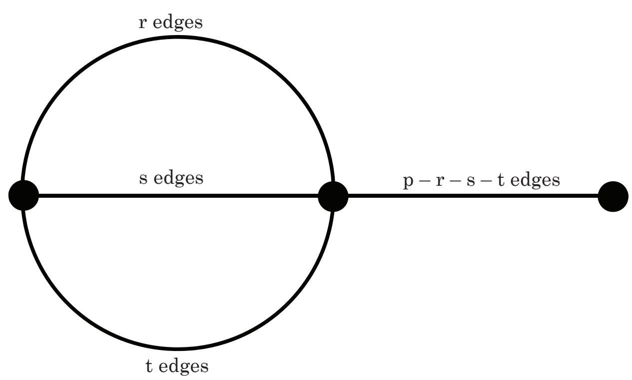


Figure 2: A graph for a regular 2^{p-2} fractional factorial design

follows that D is the design matrix of $|E|$ factors with $2^{|V|-1}$ runs defined by (12). It is easy to see that G has no K_4 minor. Hence, by virtue of Proposition 3.5, I_G is generated by quadratic binomials. □

Remark 3.10. Explicit description of binomials appearing in Theorem 3.9 is given in [18] and [10]. The set of generators of I_G consisting of quadratic binomials for a regular 2^{p-1} fractional factorial design is studied in [2].

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